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A Review Article on Role of Computer in Drug Discovery.

Moid Raza, Piyush Yadav*, and Manoj Kumar Yadav.

Prasad Institute Of Technology, Department Of Pharmacy, Jaunpur – 222001, Uttar Pradesh, India.

ABSTRACT

Now every day using Computer Aided Drug Design (CADD) technology in nanotechnology, molecular biology, biochemistry etc. The great benefits of CADD are costly in drug research and development. There is a wide range of software used in CADD, framework computing, standard window-based PBPK / PD simulation software, PKUDDS software based on APIS, JAVA, Perl and Python, CADD as well as software or software libraries. There are special techniques used in the detection of CADD, homology, molecular dynamic, reduction of molecular docking, QSAR etc. The process of drug development and drug discovery is very complex, very costly and time consuming. Accelerated due to the development of tools and methods of calculation. Over the past few years, computer aided drug design (CADD), also known as silico screening, has become a viable alternative. Various stages of drug discovery and development through various high- level factors. The CADD theater foundation includes quantum mechanics studies and molecular modeling such as structural drug-based construction; drug-based formulation; on-site searches and binding compliance based on targeted biological information. In this current update we present areas where CADD tools support the drug discovery process.

Keywords: computer aided drug design, structure based drug design, and legend based drug design, and virtual screening and molecular docking, etc.

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Corresponding author

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INTRODUCTION

Computer aided drug design (CADD) provides a variety of tools and techniques that help in various stages of drug design thus reducing research costs and drug development time. Drug discovery and the development of new drugs are a long, complex, costly, and dangerous process with a few peers in the commercial world. [1, 2, 3]. The combination of effective drug formulation and structural biology leads to the availability of novel therapeutic agents. To this end the Computer aided drug design (CADD) center works collaboratively with biologists, biophysicists and computer scientists to find new chemical businesses. CADD and bioinformatics tools provide benefits such as cost savings, marketing time, visualization of drug receptor interactions, accelerating drug discovery and development [4, 5, 6]. Computer power by combining advanced analytical techniques such as X-ray crystallography, NMR, etc. developed. The use of CADD in the pharmaceutical industry as well as many approved drugs that have shown a significant presence in CADD tools has been reported, such as: angiotensin-converting enzyme (ACE) inhibitor captopril for the treatment of hypertension[7, 8],

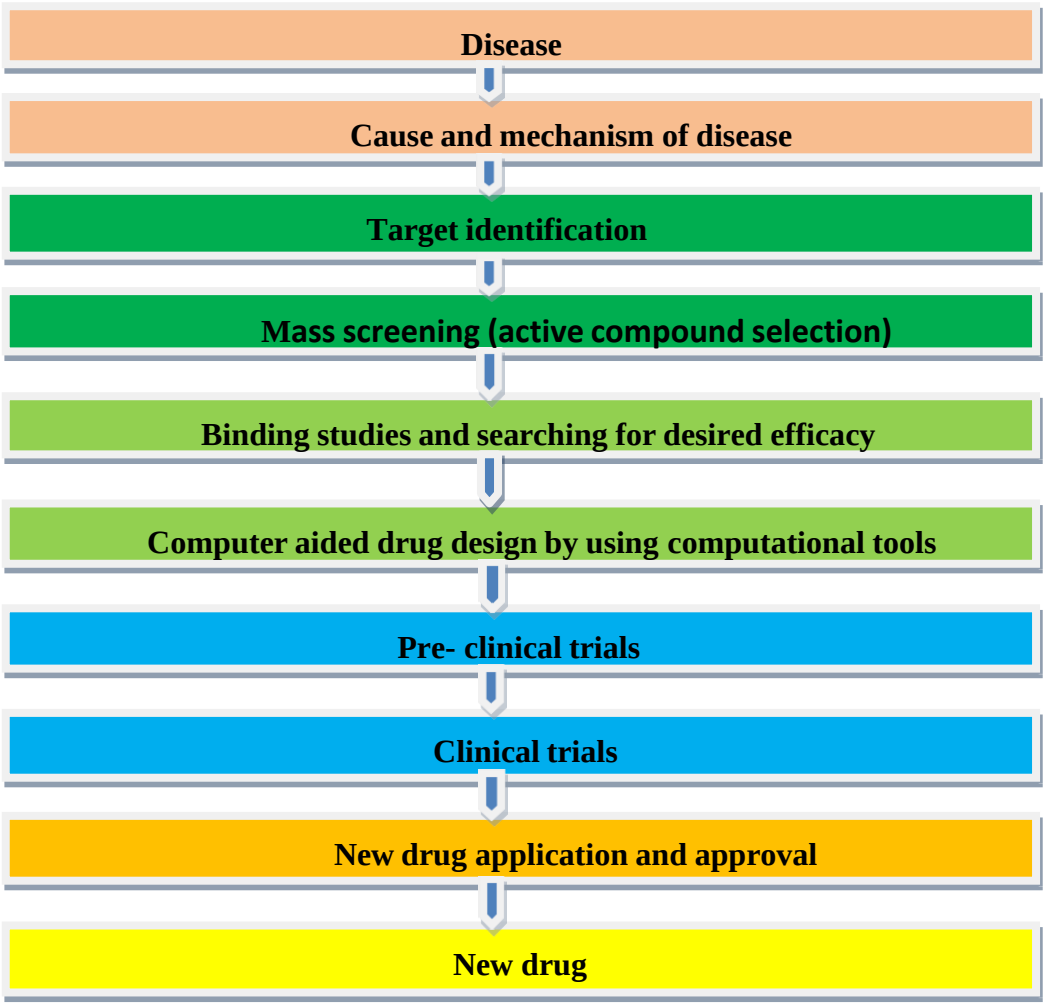

Fig: flow chart of drug discovery [9]

Major types of approaches in CADD

There are types of approaches for drug design through CADD is the following-:

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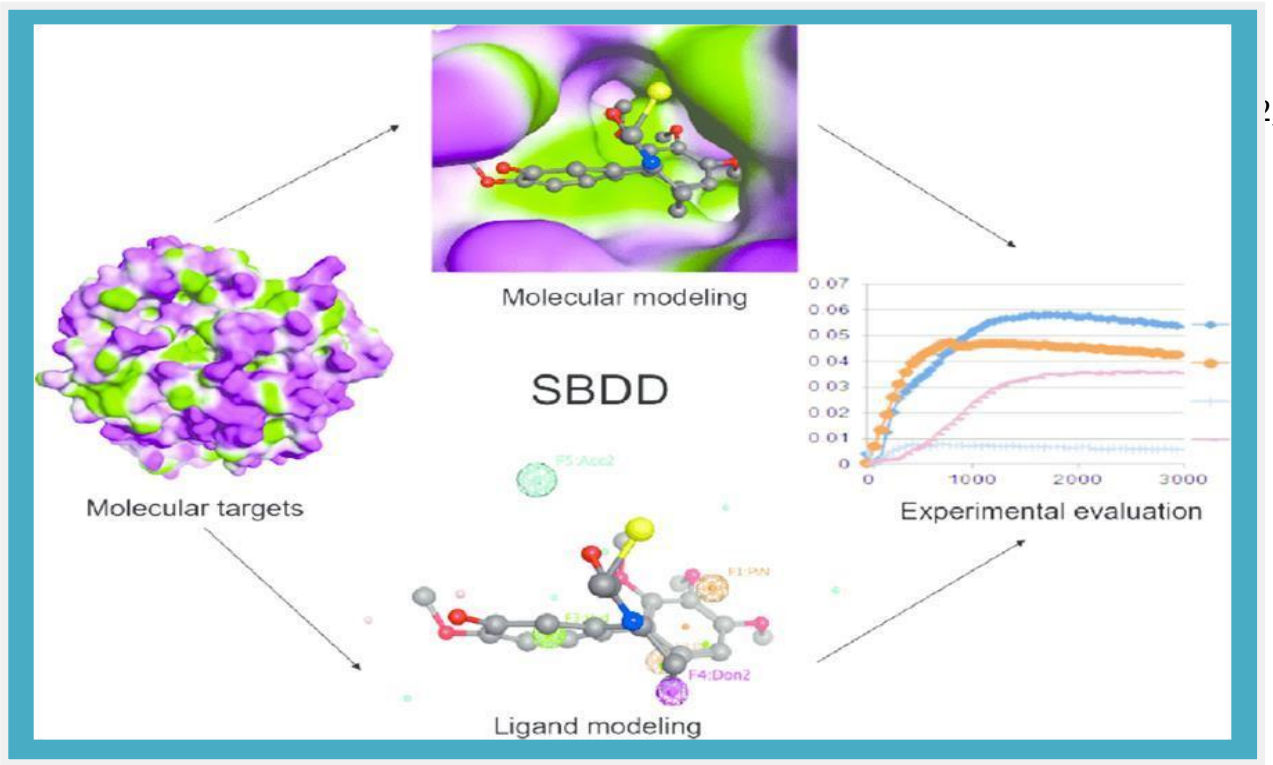
- Structure based drug design / direct approach
- Legend based drug design / indirect approach

Structure based drug design / direct approach

Structured drug-based formulations are more effective when it is part of the lead drug acquisition process. Review of J. Anted [10] states that a combination of integrated chemistry and structural- based design can lead to the harmonious integration of concentrated libraries. It is also important to consider that the structure of the drug based structure directs the acquisition of the drug, which is not a drug product but, in particular, a minimal molar affinity component of the target substance [11]. The time allotted to the structural medicine- based design process, as stated in this review, may represent a small portion of the total construction time of a marketable pharmaceutical product. Many years of research may be needed to turn lead into a drug that will work well and be tolerated by the human body. Additional years of research and development will bring medicine through clinical trials to eventually reach the market. This review is intended to provide an overview of the structural

Figure: SBDD (structure based drug design)



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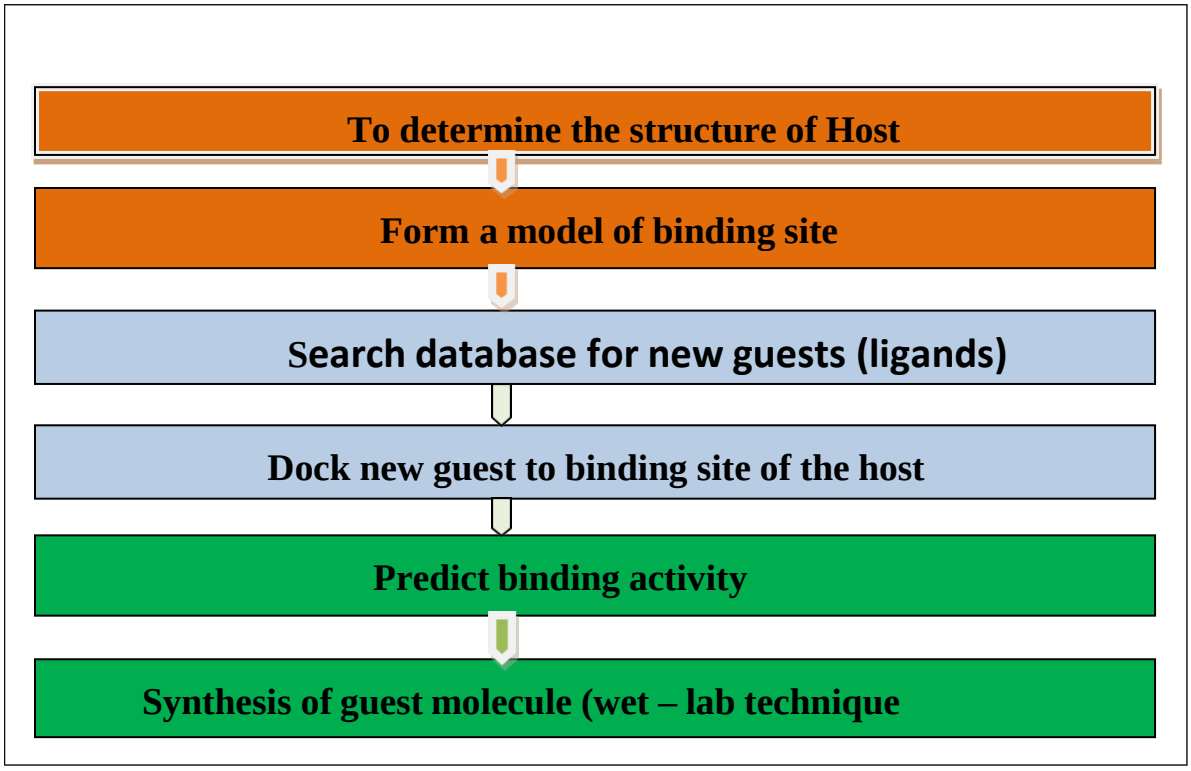

Fig steps involve in SBDD

Legend based drug design / indirect approach:-

LBDD, the 3D protein structure of the target is unknown but the myths that cover the target area are known. These myths can be used to develop a pharmacophore model or molecule with all the structural features needed to integrate a targeted functional environment. Generally based pharmacophore-based methology and quantitative work relationships (QSARs). In LBDD it is thought that similar compounds in their structure also have similar biological action and interaction with the target protein [15].

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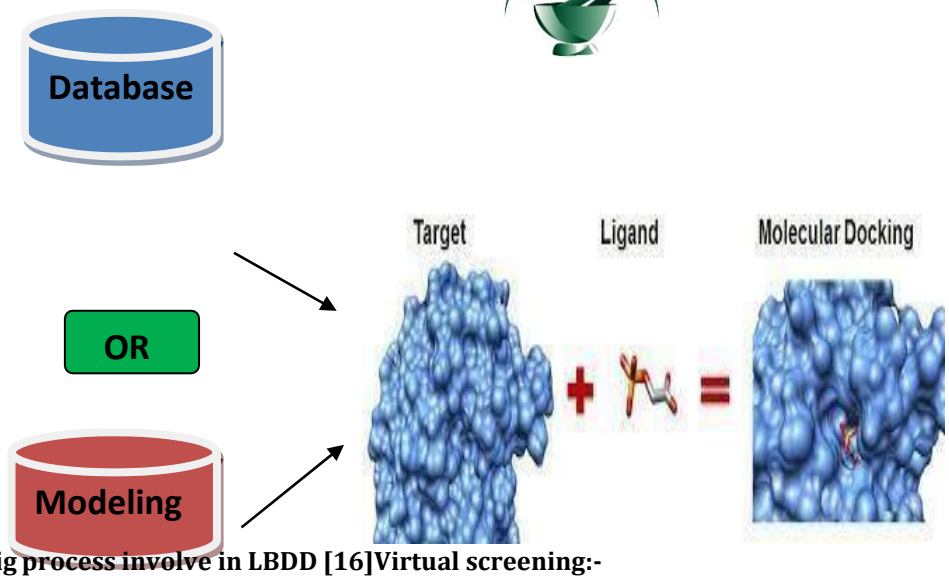

Fig process involve in LBDD [16]Virtual screening:-

Virtual exploration has been used as the most useful tool now in the day to find the most interesting bioactive compounds with the help of information about the target protein or known active myths. In recent times virtual experimentation has become known as an innovative way of testing high performance especially in terms of low cost and the chances of obtaining the most suitable novel beaten by a large filter of compound libraries[17].

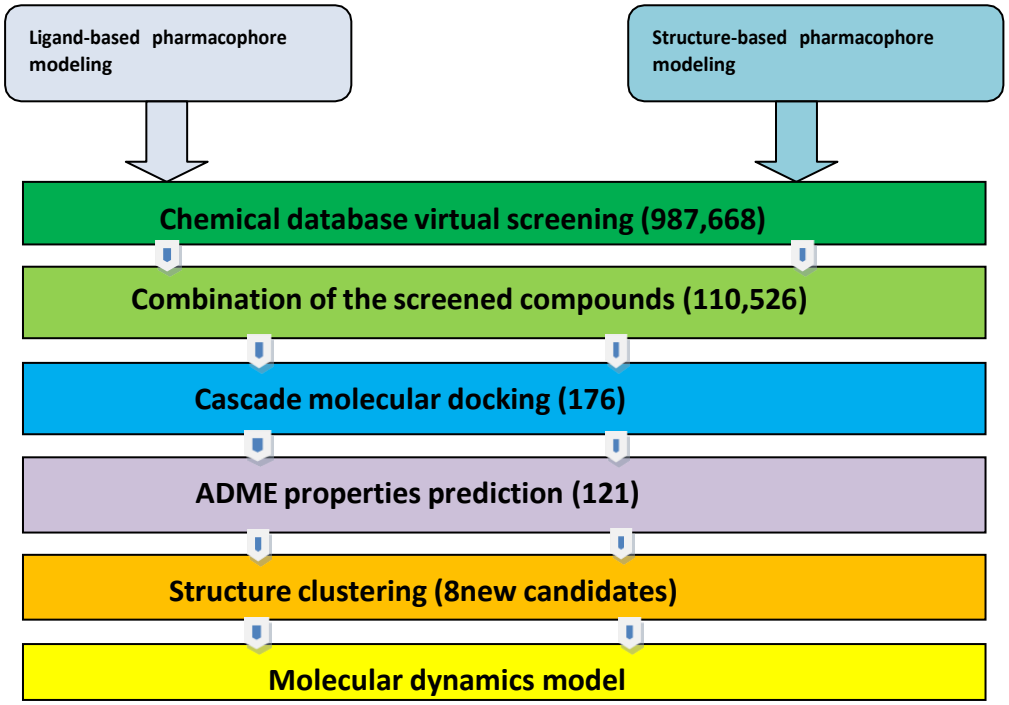

Fig steps involve virtual screening [17]Molecular Docking:-

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Molecular docking such as "lock-and-key", when a person wants to collect the correct comparative shape of a "key" that will lock the "key" (where the key to the key is the keyhole, how to lockthe key after installation, etc.). Here, protein can be thought of as "lock" and ligand can be thought of as "key". Molecular docking may be defined as the difficulty of preparation, which may explain the "most appropriate" direction of the ligand that binds to a strong protein for attention. but, as both ligand and protein stretch, the "hand-glove" connection is more appropriate than the "lock key". [18] During the detoxification process, ligand and protein adjust their alignment to achieve "optimal" and this type of concomitant change leading to complete binding is called "equilibrium- appropriate". [19] Cellular extraction is one of the most commonly used methods in SBDD due to its ability to predict, with a high degree of accuracy, the interaction of ligands of small molecules within the appropriate target binding area [20]. Following the development of algorithms that began in the 1980's, molecular docking became an important tool in drug discovery [21]. For example, research involving important cellular events, including ligand binding mechanisms and intermolecular coagulation that stabilizes a ligand-receptor compound, can be easily performed [22]. In addition, molecular docking algorithms generate predictors of binding force, providing docs of docking computers based on binding relationships of ligand-receptor complexes [23,24]. a large consensus area representing a variety of possible binding methods; (ii) accurate prediction ofinteraction strength relative to each predictable binding agreement [25]. Molecular docking systems perform these functions through a circular process, in which the ligand joint is tested for specific scoring activities. This process is repeated until it is converted to a low power solution [21, 23, 24]

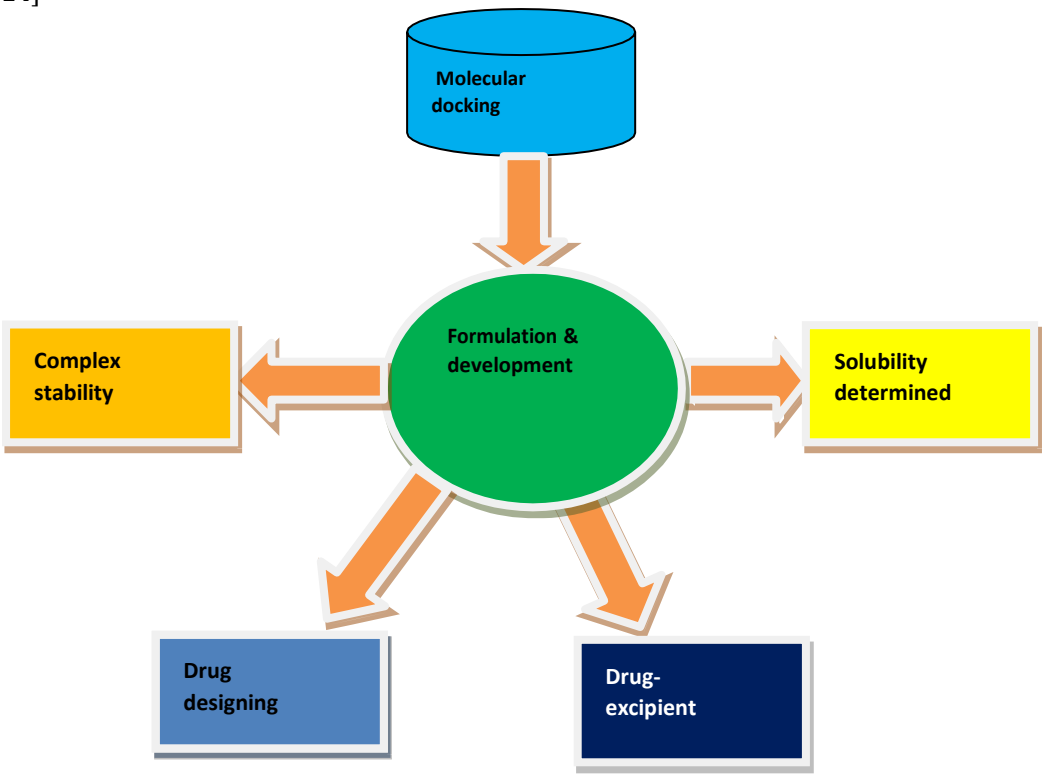

Fig: molecular Docking in Formulation and drug development

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Docking accuracy

The accuracy of the docket represents one measure of the accuracy of the docking system by measuring the ability to predict the correct ligand position in relation to what is detected by the test. [25]

CONCLUSION

News of CADD's success in drug discovery over the past few years has shown usefulness in the drug development process. CADD provides valuable information about targeted molecules, lead combinations, testing and efficacy. Recent developments such as combinatorial chemistry, various databases and new software tools are available that provide the basis for designing ligands and inhibitors that need to be specified. Different methods, design stages, docking, pharmacophore modeling, homology modeling are central to the CADD process. The use of computer chemistry is also based on understanding the three-dimensional aspects of drug interaction with receptors on a cellular basis and access to therapeutic chemicals in the design of new therapeutic agents. CADD provides information about the chemistry of chemical companies that are inaccessible through laboratory testing, cost reduction and labor. Indeed, CADD will improve research quality soon and facilitate the development of fewer drugs.

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